

Nicotinamide, 1,6-dihydro-4-hydroxy-6-oxo-

Inchi:	InChI=1S/C6H6N2O3/c7-6(11)3-2-8-5(10)1-4(3)9/h1-2H,(H2,7,11)(H2,8,9,10)
InchiKey:	ORASOOKDQIQMDZ-UHFFFAOYSA-N
Formula:	C6H6N2O3
SMILES:	NC(=O)c1c[nH]c(=O)cc1O
Mol. weight [g/mol]:	154.12
CAS:	5466-41-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.17		Crippen Method
logp	-1.302		Crippen Method
mcvol	104.910	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5466411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/116-125-4/Nicotinamide-1-6-dihydro-4-hydroxy-6-oxo.pdf>

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